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RELATIVISTIC CALCULATION OF ATOMIC N-SHELL IONIZATION BY PROTONS

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Relativistic plane-wave Born-approximation calculations of cross sections for N-shell ionization of ${}_{83}Bi$ and ${}_{92}U$ by protons with incident energies from 0.1 to 1 MeV are reported. The calculations were carried out by using Dirac-Hartree-Slater wave functions. Binding-energy change and Coulomb deflection were taken into account. The relativistic cross sections are compared with values from nonrelativistic Hartree-Slater wave functions to study the effects of relativity.

I. INTRODUCTION

Existing calculations of cross sections for Coulomb ionization of atomic inner shells by proton impact have been carried out primarily in the plane-wave Born approximation (PWBA) with screened hydrogenic wave funtions.[1-4] To go beyond the first Born approximation, the perturbed-stationary-state approach including energy-loss, Coulomb-deflection, binding, polarization and relativistic corrections (ECPSSR) was developed by Brandt and Lapicki.[5,6] To look into the effect of more realistic wave functions and of *ab initio* incorportation of relativity, we have performed a series of relativistic plane-wave Born-approximation (RPWBA) calculations of K-, L-, and M-shell ionization cross sections, using Dirac-Hartree-Slater (DHS) wave functions.[7-9] These DHS calculations have now been extended to N-subshell ionization cross sections. In this paper, we report on results for N_{1-7}-subshell ionization of $_{83}$Bi and $_{92}$U by protons and compare these new theoretical cross sections with nonrelativistic Hartree-Slater results in order to study the effects of relativity.

II. THEORETICAL METHOD

In the plane-wave Born approximation (PWBA),[1] the differential cross section for ejection of an electron from a closed atomic n shell by heavy-charged-particle impact is

$$\frac{d\sigma}{dE_f} = \frac{4\pi}{\hbar^2} Z_1^2 e^4 \frac{M_1}{E_1} (2j_n+1) \int_{q_{min}}^{q_{max}} \frac{dq}{q^3} |F_{fi}(q)|^2 . \qquad (1)$$

Here, E_f is the kinetic energy of the ejected electron, $\hbar q$ is the momentum transferred to that electron, and Z_1, M_1, and E_1 are the charge, mass, and initial kinetic energy of the projectile, respectively; $F_{fi}(q)$ is the relativistic form factor. The exact limits of the momentum transfer[5,7] were used in the present calculations.

To take into account the effect caused by the presence of the slow charged projectile in the vicinity of the nucleus during the collision, the N-shell binding energy of the united atom (i.e. of the atom with atomic number Z_2+1 in the case of proton impact) was used in these calculations. This increase in binding energy tends to reduce the ionization cross section.

The effect of the Coulomb repulsion between the projectile and the target nucleus on the N-subshell ionization was taken into account by applying a correction factor to the cross section calculated for a straight-line projectile path.[10,11] The differential cross sections including the Coulomb-deflection correction can be written as[10,11]

$$\left(\frac{d\sigma_n}{dE_f}\right)^{C} = \left(\frac{d\sigma_n}{dE_f}\right)^{PWBA} \exp\left(-\pi d q_0\right), \qquad (2)$$

where

$$q_0 = (U_n + E_f)/v_1 \quad . \qquad (3)$$

Here, U_n is the binding energy of an n-shell electron, d is the half-distance between the collision partners at closest approach, and v_1 is the initial projectile speed.

A general computer program, written for calculating relativistic PWBA (RPWBA) ionization cross sections with DHS wave functions, was employed to evaluate the N_1-subshell Coulomb ionization cross sections. The atomic form factors were calculated with neutral-atom DHS wave functions.[12,13] The form-factor integrals were computed by two successive fast Fourier transforms.[14] The detailed numerical procedure is described in Ref. 7.

Nonrelativistic Hartree-Slater (HS) wave functions were generated with the same DHS program by multiplying the speed of light by a factor of 1,000 so as to simulate the nonrelativistic limit.[15,16] The same general program for evaluating relativistic ionization cross sections was then employed to calculate the Hartree-Slater (HS) PWBA cross sections for comparison with the relativistic results. Identical N_1-subshell binding energies from relativistic theory[13] were used in both DHS and HS calculations.

III. RESULTS AND DISCUSSION

In Table I we list the N_1-, N_2-, and N_3-subshell ionization cross sections calculated from the DHS model for $_{83}$Bi and $_{92}$U under proton impact with incident energies between 0.1 and 1 MeV. Results for the $N_{4,5}$ and $N_{6,7}$ subshells are listed in Table II. The theoretical values listed in Tables I and II are relativistic plane-wave Born cross sections (RPWBA) as well as cross sections corrected for binding and Coulomb-deflection effects (RPWBA-BC). The plane-wave Born cross sections from DHS and HS wave functions are compared in Figs. 1 and 2.

The binding correction reduces the N_i-subshell ionization cross sections by ~15-25% at E_1=0.1 MeV and by ~8% at E_1=1 MeV. Coulomb deflection leads to a reduction of N_i- subshell ionization cross sections by as much as a factor of 2 at E_1=0.1 MeV but by only 2.8% at E_1=1 MeV.

Relativistic effects on the K-, L-, and M-subshell ionization cross sections have previously been found to be quite important.[7,8,16-18] For the N shell, we find substantial relativistic effects in the lowest two subshells. The N_1 ionization cross section is enhanced by as much as 50% for $_{83}$Bi and 80% for $_{92}$U if relativity is included. The N_2 ionization cross section is enhanced by 35% for Bi and 45% for U. On the other hand, the ionization cross sections for the outer subshells N_3 through N_7 are affected by only a few percent when relativity is taken into account. The effect of relativity on the total N-shell ionization cross section can therefore be expected to be minimal, since the $N_{6,7}$-subshell cross sections are one to two orders of magnitude larger than the $N_{1,2}$ cross sections.

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TABLE I. Relativistic plane-wave Born-approximation cross sections (RPWBA) (in barns), calculated from Dirac-Hartree-Slater wave functions for $N_{1,2,3}$-subshell ionization of Bi and U by protons of energy E_1(in MeV). Numbers in parentheses indicate powers of 10, e.g., 1.05(3)=1.05x10^3.

	N_1		N_2		N_3	
E_1	RPWBA	RPWBA-BC	RPWBA	RPWBA-BC	RPWBA	RPWBA-BC
			$_{83}Bi$			
0.1	1.05(3)	3.92(2)	2.71(3)	9.83(2)	1.08(4)	4.51(3)
0.2	4.71(3)	2.47(3)	1.28(4)	7.62(3)	4.16(4)	2.70(4)
0.3	1.42(4)	9.16(3)	2.59(4)	1.81(4)	7.57(4)	5.59(4)
0.4	2.48(4)	1.80(4)	3.83(4)	2.91(4)	1.08(5)	8.48(4)
0.5	3.45(4)	2.68(4)	4.91(4)	3.92(4)	1.36(5)	1.11(5)
0.6	4.27(4)	3.47(4)	5.80(4)	4.79(4)	1.59(5)	1.34(5)
0.7	4.93(4)	4.13(4)	6.50(4)	5.51(4)	1.77(5)	1.53(5)
0.8	5.45(4)	4.67(4)	7.05(4)	6.09(4)	1.91(5)	1.68(5)
0.9	5.85(4)	5.11(4)	7.46(4)	6.55(4)	2.02(5)	1.80(5)
1.0	6.15(4)	5.46(4)	7.78(4)	6.92(4)	2.10(5)	1.89(5)
			$_{92}U$			
0.1	3.06(2)	2.53(2)	4.38(2)	1.09(2)	1.77(3)	5.47(2)
0.2	6.49(2)	3.34(2)	1.82(3)	9.38(2)	7.60(3)	4.41(3)
0.3	1.78(3)	1.03(3)	4.54(3)	2.89(3)	1.72(4)	1.19(4)
0.4	4.14(3)	2.71(3)	8.09(3)	5.71(3)	2.84(4)	2.14(4)
0.5	7.20(3)	5.14(3)	1.20(4)	8.99(3)	3.99(4)	3.17(4)
0.6	1.05(4)	7.91(3)	1.57(4)	1.23(4)	5.11(4)	4.20(4)
0.7	1.37(4)	1.08(4)	1.93(4)	1.56(4)	6.14(4)	5.17(4)
0.8	1.67(4)	1.36(4)	2.24(4)	1.87(4)	7.06(4)	6.06(4)
0.9	1.94(4)	1.62(4)	2.53(4)	2.14(4)	7.86(4)	6.86(4)
1.0	2.18(4)	1.85(4)	2.76(4)	2.38(4)	8.54(4)	7.55(4)

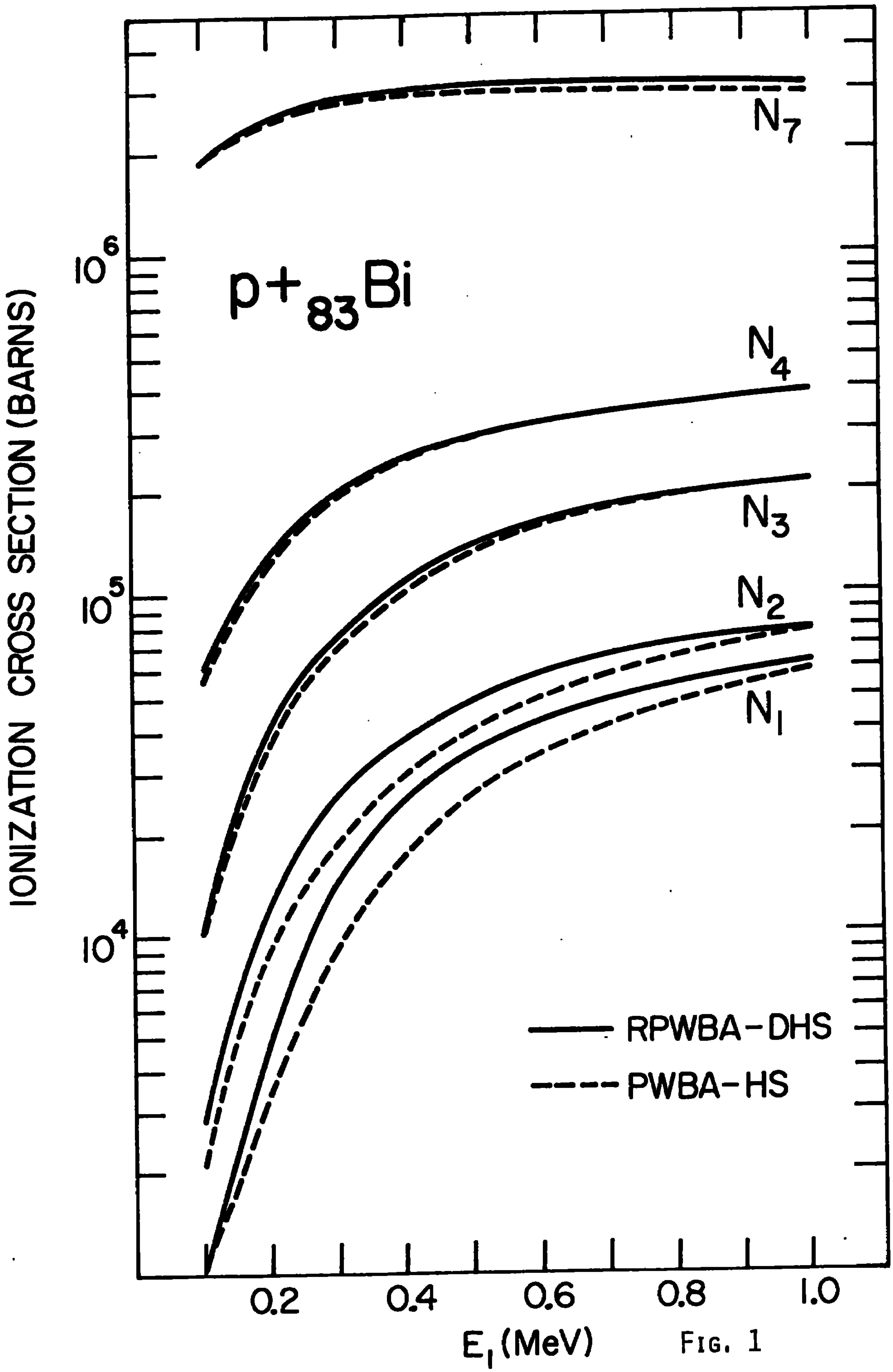
TABLE II. Relativistic plane-wave Born-approximation cross sections (RPWBA) (in barns), calculated from Dirac-Hartree-Slater wave functions for $N_{4,5}$- and $N_{6,7}$-subshell ionization of Bi and U by protons of energy E_1 (in MeV).

	N_4		N_5		N_6		N_7	
E_1	RPWBA	RPWBA-BC	RPWBA	RPWBA-BC	RPWBA	RPWBA-BC	RPWBA	RPWBA-BC
				$_{83}Bi$				
0.1	6.04(4)	3.17(4)	9.76(4)	5.20(4)	1.29(6)	8.07(5)	1.84(6)	1.16(6)
0.2	1.32(5)	9.24(4)	2.29(5)	1.60(5)	1.79(6)	1.36(6)	2.54(6)	1.93(6)
0.3	1.99(5)	1.53(5)	3.49(5)	2.70(5)	2.01(6)	1.63(6)	2.83(6)	2.31(6)
0.4	2.52(5)	2.04(5)	4.37(5)	3.57(5)	2.12(6)	1.78(6)	2.98(6)	2.51(6)
0.5	2.92(5)	2.45(5)	5.01(5)	4.24(5)	2.18(6)	1.87(6)	3.07(6)	2.64(6)
0.6	3.21(5)	2.76(5)	5.47(5)	4.73(5)	2.22(6)	1.93(6)	3.12(6)	2.72(6)
0.7	3.43(5)	3.00(5)	5.79(5)	5.10(5)	2.23(6)	1.97(6)	3.13(6)	2.77(6)
0.8	3.58(5)	3.17(5)	6.02(5)	5.37(5)	2.23(6)	1.99(6)	3.13(6)	2.79(6)
0.9	3.69(5)	3.31(5)	6.19(5)	5.58(5)	2.22(6)	2.00(6)	3.11(6)	2.80(6)
1.0	3.76(5)	3.41(5)	6.28(5)	5.71(5)	2.21(6)	2.00(6)	3.09(6)	2.80(6)
				$_{92}U$				
0.1	1.03(4)	4.06(3)	1.80(4)	7.46(3)	1.64(5)	8.84(4)	2.41(5)	1.32(5)
0.2	2.96(4)	1.92(4)	4.98(4)	3.27(4)	3.02(5)	2.20(5)	4.37(5)	3.22(5)
0.3	4.94(4)	3.66(4)	8.67(4)	6.46(4)	3.99(5)	3.19(5)	5.73(5)	4.61(5)
0.4	6.85(4)	5.42(4)	1.22(5)	9.72(4)	4.72(5)	3.94(5)	6.75(5)	5.66(5)
0.5	8.58(4)	7.05(4)	1.54(5)	1.27(5)	5.29(5)	4.53(5)	7.54(5)	6.48(5)
0.6	1.01(5)	8.53(4)	1.80(5)	1.53(5)	5.73(5)	4.99(5)	8.17(5)	7.14(5)
0.7	1.14(5)	9.83(4)	2.02(5)	1.76(5)	6.10(5)	5.38(5)	8.69(5)	7.69(5)
0.8	1.25(5)	1.10(5)	2.21(5)	1.95(5)	6.40(5)	5.70(5)	9.08(5)	8.12(5)
0.9	1.35(5)	1.20(5)	2.37(5)	2.11(5)	6.63(5)	5.96(5)	9.42(5)	8.49(5)
1.0	1.43(5)	1.28(5)	2.50(5)	2.25(5)	6.82(5)	6.17(5)	9.68(5)	8.78(5)

Figure Captions

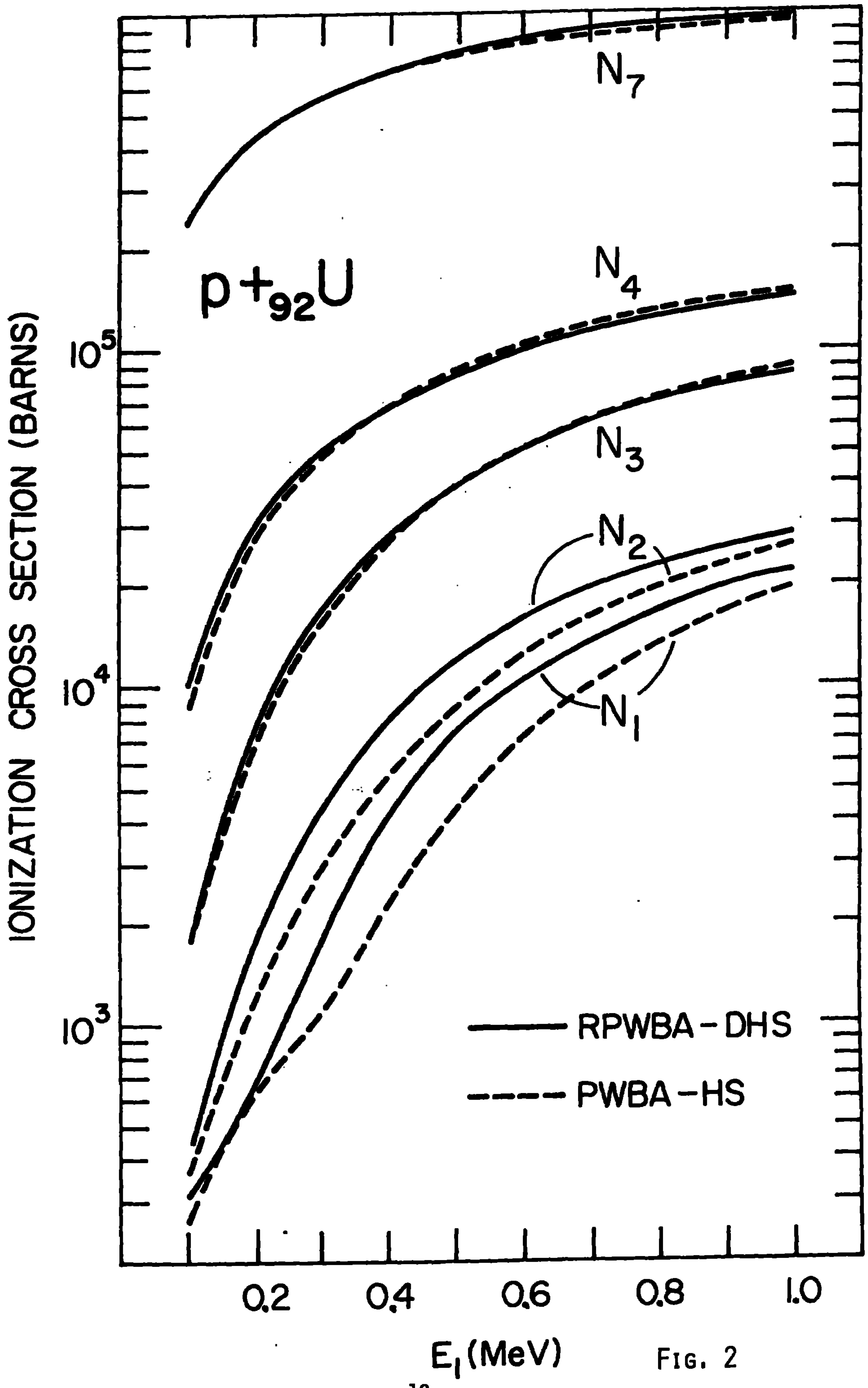
FIG. 1. Cross sections for N_1-subshell ionization of Bi by proton bombardment, as functions of incident-proton energy. Results of the present relativistic plane-wave Born-approximation calculations from Dirac-Hartree-Slater wave functions (solid curves) are compared with cross sections computed nonrelativistically from Hartree-Slater wave functions (dashed curves).

FIG. 2. Cross sections for N_1-subshell ionization of U by protons, as functions of incident proton energy. Curves are identifed in the caption of Fig. 1.



IONIZATION CROSS SECTION (BARNS)
10^6
10^5
10^4
$p + {}_{83}Bi$
N_7
N_4
N_3
N_2
N_1
RPWBA-DHS
PWBA-HS
0.2
0.4
0.6
0.8
1.0
E_1 (MeV)

FIG. 1



p + $_{92}$U
N_7
N_4
N_3
N_2
N_1
IONIZATION CROSS SECTION (BARNS)
10^5
10^4
10^3
RPWBA - DHS
PWBA - HS
0.2
0.4
0.6
0.8
1.0
E_1 (MeV)

FIG. 2